

RECOVERING A PHYLOGENETIC TREE USING
PAIRWISE CLOSURE OPERATIONS

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RECOVERING A PHYLOGENETIC TREE USING PAIRWISE CLOSURE OPERATIONS

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ABSTRACT. A fundamental task in evolutionary biology is the amalgamation of a collection \mathcal{P} of leaf-labelled trees into a single parent tree. A desirable feature of any such amalgamation is that the resulting tree preserves all of the relationships described by the trees in \mathcal{P} . For unrooted trees, deciding if there is such a tree is NP-complete. However, two polynomial-time approaches that sometimes provide a solution to this problem involve the computation of the semi-dyadic closure and split closure of a set of quartets that underlies \mathcal{P} . In this paper we show that if a leaf-labelled tree T can be recovered from the semi-dyadic closure of some set \mathcal{Q} of quartet subtrees of T , then T can also be recovered from the split-closure of \mathcal{Q} . Furthermore, we show that the converse of this result does not hold, and resolve a closely related question posed in [1].

1. INTRODUCTION

A *binary phylogenetic (X)-tree* is an unrooted tree in which every interior vertex has degree three and whose leaf set is X . In evolutionary biology, X is commonly a set of species and a binary phylogenetic X -tree is used to represent the evolutionary relationships between the species in X .

A natural and fundamental task in evolutionary biology is to amalgamate binary phylogenetic trees that classify different, but overlapping, sets of species into a single parent tree. This single parent tree is called a *supertree* and ways to perform such tasks are called *supertree methods*. A desirable property of any supertree method is that, if possible, the resulting supertree ‘displays’ all of the evolutionary relationships of the input trees. More precisely, let T and T' be binary phylogenetic trees with leaf sets X and X' , respectively. Then T' *displays* T if $X \subseteq X'$ and, up to suppressing degree two vertices, T is the minimal subtree of T' that connects the elements of X . In general, a binary phylogenetic tree T' *displays* a collection \mathcal{P} of binary phylogenetic trees if T' displays each tree in \mathcal{P} . This desirable property of a supertree method leads to the following algorithmic problem.

Problem: TREE COMPATIBILITY

Instance: A collection \mathcal{P} of binary phylogenetic trees.

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Question: Does there exist a binary phylogenetic tree that displays each of the trees in \mathcal{P} and, if so, can we construct such a binary phylogenetic tree?

In general, this problem is NP-complete [5]. However, there are a number of polynomial-time approaches to this problem that may provide a solution. Two of these approaches are based on the closure operators ‘semi-dyadic closure’ and ‘split closure’. The former is associated with a collection of quartets and the latter is associated with a collection of splits.

A *quartet* is a binary phylogenetic tree with four leaves. The quartet with leaves a, b, c, d is denoted $ab|cd$ if the path from a to b does not intersect the path from c to d . A *split* of X , also called an X -*split*, is a partition of X into two non-empty subsets. Deleting any edge of a binary phylogenetic X -tree induces a split of X , namely the bipartition of X whose parts are the vertex sets of the resulting components. For a binary phylogenetic X -tree \mathcal{T} , let $\mathcal{Q}(\mathcal{T})$ denote the set of quartets displayed by \mathcal{T} and let $\Sigma(\mathcal{T})$ denote the set of splits of X induced by the interior edges of \mathcal{T} . It is well-known that \mathcal{T} can be (efficiently) reconstructed from either $\mathcal{Q}(\mathcal{T})$ or $\Sigma(\mathcal{T})$. This means that possible solutions to TREE COMPATIBILITY can be sought by ‘encoding’ the input trees either as a set \mathcal{Q} of quartets or as a set Σ of splits, and then using these encodings either to construct an encoding of a binary phylogenetic tree that displays each of the original trees or to determine that no such tree exists. Two possible approaches in this regard are to compute the semi-dyadic closure of \mathcal{Q} in case the encoding is done in terms of quartets or the split closure of Σ in case the encoding is done in terms of splits [3, 4]. The precise definitions are given in Section 2, but, roughly speaking, semi-dyadic closure and split closure are the end result of repeatedly applying a pairwise inference rule to collections of quartets or splits, respectively.

Quartets themselves can be encoded by splits—simply take the splits induced by the interior edges of the quartets—and so it is natural to ask how the semi-dyadic closure and split closure of a set \mathcal{Q} of quartets are related. For the split closure of \mathcal{Q} , we view \mathcal{Q} as a set of splits. In Section 3, we consider the relationship between the semi-dyadic closure and split closure of \mathcal{Q} when one or the other recovers a binary phylogenetic tree. In particular, we prove the following theorem.

Theorem 1.1. *Let \mathcal{T} be a binary phylogenetic tree and let \mathcal{Q} be a subset of $\mathcal{Q}(\mathcal{T})$. If the semi-dyadic closure of \mathcal{Q} equals $\mathcal{Q}(\mathcal{T})$, then the split-closure of \mathcal{Q} equals $\Sigma(\mathcal{T})$.*

Essentially, Theorem 1.1 states that if a binary phylogenetic tree \mathcal{T} can be recovered from a subset \mathcal{Q} of $\mathcal{Q}(\mathcal{T})$ using the semi-dyadic closure of \mathcal{Q} , then \mathcal{T} can also be recovered from \mathcal{Q} using the split-closure of \mathcal{Q} . Surprisingly, the converse of Theorem 1.1 is not true, a fact that we will also establish in Section 3.

The original motivation for Theorem 1.1 arose from an open question in [1, Remark 4] which relates semi-dyadic closure to minimum-sized sets of quartets that define a binary phylogenetic tree. In the last section, we resolve this question.

We end this section by noting that, throughout this paper, X is a finite set, and the notation and terminology follows [4].

2. SEMI-DYADIC CLOSURE AND SPLIT CLOSURE

The *semi-dyadic closure* of an arbitrary collection \mathcal{Q} of quartets, denoted $\text{scl}_2(\mathcal{Q})$, is the minimal set of quartets that contains \mathcal{Q} and that has the property that if $ab|cd, ac|de \in \text{scl}_2(\mathcal{Q})$, then

$$ab|ce, ab|de, bc|de \in \text{scl}_2(\mathcal{Q}).$$

The significance of this pairwise inference rule is highlighted in Proposition 2.1 [2].

Proposition 2.1. *Let \mathcal{Q} be a set of quartets and let \mathcal{T} be a binary phylogenetic tree. Then \mathcal{T} displays \mathcal{Q} if and only if \mathcal{T} displays $\text{scl}_2(\mathcal{Q})$.*

To describe split closure, we first need some additional definitions. A *partial split* of X or, more briefly, *partial X -split* is a partition of a subset of X into two non-empty subsets. If these two subsets are A and B , we denote the partial X -split by $A|B$ or, equivalently, by $B|A$. A partial X -split $A|B$ is a (*full*) X -split if $A \cup B = X$. We say that a partial X -split $A'|B'$ *extends* a partial X -split $A|B$ if either $A \subseteq A'$ and $B \subseteq B'$, or $B \subseteq A'$ and $A \subseteq B'$. In general, a collection Σ' of partial X -splits *extends* a collection Σ of partial X -splits if, for each $\sigma \in \Sigma$, there is an element $\sigma' \in \Sigma'$ such that σ' extends σ . Furthermore, if, for all $\sigma \in \Sigma$, the set Σ contains no partial X -split that extends σ , then we say that Σ is *irreducible*.

The *split closure* of an arbitrary collection Σ of partial X -splits, denoted $\text{spcl}(\Sigma)$, is the minimal irreducible set of partial X -splits that extends Σ and has the following property:

- If $A_1|B_1$ and $A_2|B_2$ are elements of Σ that satisfy
- (1) $\emptyset \notin \{A_1 \cap A_2, A_1 \cap B_2, B_1 \cap B_2\}$ and $B_1 \cap A_2 = \emptyset$,
- then there are elements of $\text{spcl}(\Sigma)$ that extend $(A_1 \cup A_2)|B_1$ and $A_2|(B_1 \cup B_2)$.

The fact that there is a unique minimal irreducible set of partial X -splits that has this property and extends Σ is shown in [3].

The next lemma and corollary will be used in the proof of Theorem 1.1. A binary phylogenetic X -tree \mathcal{T} *displays* a partial X -split σ if there is an X -split in $\Sigma(\mathcal{T})$ that extends σ . In general, \mathcal{T} *displays* a collection Σ of partial X -splits if \mathcal{T} displays each member of Σ . Furthermore, for a partial X -split $A|B$, let

$$\mathcal{Q}(A|B) = \{aa'|bb' : a, a' \in A; b, b' \in B; a \neq a'; b \neq b'\}$$

and, for a set Σ of partial X -splits, let $\mathcal{Q}(\Sigma) = \bigcup_{A|B \in \Sigma} \mathcal{Q}(A|B)$. Observe that, for all binary phylogenetic trees \mathcal{T} , we have $\mathcal{Q}(\Sigma(\mathcal{T})) = \mathcal{Q}(\mathcal{T})$. Part (i) of Lemma 2.2 is due to Meacham [2] and part (ii) is proved in [3].

Lemma 2.2. *Let Σ be a set of partial X -splits. Then*

- (i) *A binary phylogenetic tree \mathcal{T} displays Σ if and only if \mathcal{T} displays $\text{spcl}(\Sigma)$.*
- (ii) *If there exists a binary phylogenetic tree that displays Σ , then $\text{scl}_2(\mathcal{Q}(\Sigma)) \subseteq \mathcal{Q}(\text{spcl}(\Sigma))$.*

An immediate consequence of Lemma 2.2 is Corollary 2.3

Corollary 2.3. *Let T be a phylogenetic tree and let $\mathcal{Q} \subseteq \mathcal{Q}(T)$. If $\text{scl}_2(\mathcal{Q}) = \mathcal{Q}(T)$, then $\mathcal{Q}(\text{spcl}(\mathcal{Q})) = \mathcal{Q}(T)$.*

3. PROOF OF THEOREM 1.1

Before proving Theorem 1.1, we require one further concept. Let T be a binary phylogenetic tree and let e be an interior edge of T . A quartet $q \in \mathcal{Q}(T)$ *distinguishes* e if e is the unique interior edge of T for which the quartet q is extended by the X -split in $\Sigma(T)$ induced by e . Furthermore, a partial X -split σ *distinguishes* e if there is a quartet in $\mathcal{Q}(\sigma)$ that distinguishes e .

Proof of Theorem 1.1. Let T be a binary phylogenetic tree and let \mathcal{Q} be a subset of $\mathcal{Q}(T)$, and suppose that $\text{scl}_2(\mathcal{Q}) = \mathcal{Q}(T)$. Evidently, the theorem holds if T has exactly one interior edge. Therefore we may assume that T has at least two interior edges. Now assume that $\text{spcl}(\mathcal{Q}) \neq \Sigma(T)$.

We first show that there exists a partial X -split in $\text{spcl}(\mathcal{Q})$ that distinguishes an interior edge and is not full. Let e be an interior edge of T and let q be a quartet in $\mathcal{Q}(T)$ that distinguishes e . Then, by Corollary 2.3, $q \in \mathcal{Q}(\text{spcl}(\mathcal{Q}))$ and so there exists a partial X -split σ in $\text{spcl}(\mathcal{Q})$ that extends q . This means that σ distinguishes e and so it follows that, for all interior edges e of T , there is a partial X -split in $\text{spcl}(\mathcal{Q})$ that distinguishes e . Furthermore, not all of these partial X -splits are full, for otherwise $\text{spcl}(\mathcal{Q}) = \Sigma(T)$.

Let $\sigma_1 = A_1|B_1$ be a partial X -split in $\text{spcl}(\mathcal{Q})$ that is not full and distinguishes the interior edge e_1 of T . Since σ_1 is not full, there exists an element $x \in X$ with $x \notin A_1 \cup B_1$. By considering the interior edge(s) of T that are adjacent to e_1 and using Corollary 2.3, it is easily seen that there exists a quartet $xb|cd$ in $\mathcal{Q}(\text{spcl}(\mathcal{Q}))$ that distinguishes an interior edge of T adjacent to e_1 with $b, c \in A_1$ and $d \in B_1$. Let $\sigma_2 = A_2|B_2$ be a partial X -split in $\text{spcl}(\mathcal{Q})$ that extends $xb|cd$. Clearly, $\sigma_1 \neq \sigma_2$. Without loss of generality, we may assume that $x, b \in A_2$ and $c, d \in B_2$. As T displays σ_1 and σ_2 , and $\emptyset \notin \{A_1 \cap A_2, A_1 \cap B_2, B_1 \cap B_2\}$, we must have $B_1 \cap A_2 = \emptyset$ (this is a well-known property of binary phylogenetic trees, see [4]). By the definition of split closure, this means that there is an element of $\text{spcl}(\mathcal{Q})$ that extends $(A_1 \cup A_2)|B_1$. But then this element strictly extends σ_1 , contradicting the irreducibility of $\text{spcl}(\Sigma)$. This completes the proof of the theorem. \square

The converse of Theorem 1.1 holds if T has at most six leaves, but fails in general. To see this, consider the binary phylogenetic tree T shown in Fig. 1 and the set $\mathcal{Q} = \{26|57, 16|47, 15|34, 15|23, 14|37\}$ of quartets. Now $\mathcal{Q} \subseteq \mathcal{Q}(T)$, and it is easily verified that $\text{spcl}(\mathcal{Q}) = \Sigma(T)$. However,

$$\text{scl}_2(\mathcal{Q}) = \mathcal{Q} \cup \{16|37, 46|37, 16|34, 15|37, 45|37, 15|47\} \neq \mathcal{Q}(T).$$

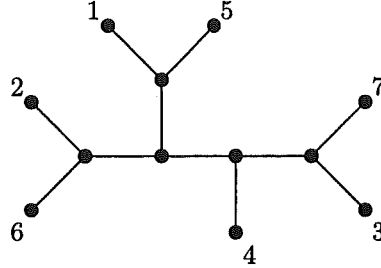


FIGURE 1. A binary phylogenetic tree.

4. TIGHT SETS

Let \mathcal{P} be a collection of binary phylogenetic trees. We say that \mathcal{P} defines a binary phylogenetic tree T if T displays \mathcal{P} and T is the only such tree with this property. Furthermore, the *excess* of \mathcal{P} , denoted $\text{exc}(\mathcal{P})$, is the quantity

$$\text{exc}(\mathcal{P}) = |\mathcal{L}(\mathcal{P})| - 3 - \sum_{T \in \mathcal{P}} i(T),$$

where $\mathcal{L}(\mathcal{P})$ is the union of the leaf sets of trees in \mathcal{P} and $i(T)$ is the number of interior edges of T . For a binary phylogenetic tree T , we say that \mathcal{P} is *T -tight* if \mathcal{P} defines T and $\text{exc}(\mathcal{P}) = 0$. In particular, if a collection \mathcal{Q} of quartets is T -tight, then \mathcal{Q} has size $|\mathcal{L}(T)| - 3$, the smallest sized subset of $\mathcal{Q}(T)$ that defines T . Loosely speaking, a collection of binary phylogenetic trees is T -tight if it contains the absolute minimum amount of information that is required to recover a binary phylogenetic tree T .

It is shown in [1, Theorem 3] that if \mathcal{P} is a collection of binary phylogenetic trees that defines a binary phylogenetic tree T and contains a T -tight subset \mathcal{P}' , then

$$\text{scl}_2 \left(\bigcup_{T' \in \mathcal{P}} \mathcal{Q}(T') \right) = \mathcal{Q}(T).$$

Moreover, in the remark directly following this theorem, it is stated that the converse of this result does not hold for arbitrary collections \mathcal{P} of binary phylogenetic trees. However, the authors also state that they do not know if this is the case when \mathcal{P} consists of quartets. In other words, the following question remained unanswered: if T is a binary phylogenetic tree and $\mathcal{Q} \subseteq \mathcal{Q}(T)$ with $\text{scl}_2(\mathcal{Q}) = \mathcal{Q}(T)$, does it follow that $\mathcal{Q}(T)$ contains a T -tight subset? Observe that \mathcal{Q} satisfies the assumptions of Theorem 1.1. We conclude this paper by providing an example which shows that this is not necessarily the case.

Let T be the binary phylogenetic tree shown in Fig. 2(a) and let

$$\mathcal{Q} = \{14|56, 15|36, 23|45, 12|36\}.$$

Note that $\mathcal{Q} \subseteq \mathcal{Q}(T)$. It is straightforward to check that $\text{scl}_2(\mathcal{Q}) = \mathcal{Q}(T)$. Now, each quartet in $\mathcal{Q} - \{15|36\}$ distinguishes a distinct interior edge of T , while $15|36$ does not distinguish any interior edge of T . This means that the only possibility for a T -tight subset of \mathcal{Q} is $\mathcal{Q} - \{15|36\}$ as every interior edge of T needs to be



FIGURE 2. Two binary phylogenetic trees.

distinguished by a quartet in \mathcal{Q} (see [4, Theorem 6.8.7]). But the binary phylogenetic tree shown in Fig. 2(b) also displays $\mathcal{Q} - \{15|36\}$. Thus $\mathcal{Q} - \{15|36\}$ does not define \mathcal{T} and so \mathcal{Q} does not contain a \mathcal{T} -tight subset.

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